Ye Xu

List of Publications by Year
in descending order

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130 papers	13,981 citations	36271 51 h-index	20343 116 g-index
137 all docs	137 docs citations	137 times ranked	13543 citing authors

#	Article	IF	Citations
1	A Highâ€Performance Nonfused Wideâ€Bandgap Acceptor for Versatile Photovoltaic Applications. Advanced Materials, 2022, 34, e2108090.	11.1	71
2	Mapping the energy level alignment at donor/acceptor interfaces in non-fullerene organic solar cells. Nature Communications, 2022, 13, 2046.	5.8	41
3	Design of ultranarrow-bandgap acceptors for efficient organic photovoltaic cells and highly sensitive organic photodetectors. Journal of Energy Chemistry, 2022, 72, 388-394.	7.1	10
4	Thermal stability and protective properties of phenylphosphonic acid on Cu(111). Applied Surface Science, 2022, 600, 154036.	3.1	1
5	Organic photovoltaic cells with high efficiencies for both indoor and outdoor applications. Materials Chemistry Frontiers, 2021, 5, 893-900.	3.2	32
6	Recent progress in reducing voltage loss in organic photovoltaic cells. Materials Chemistry Frontiers, 2021, 5, 709-722.	3.2	41
7	Design of ultra-high luminescent polymers for organic photovoltaic cells with low energy loss. Chemical Communications, 2021, 57, 9132-9135.	2.2	12
8	Quadrupole Moment Induced Morphology Control Via a Highly Volatile Small Molecule in Efficient Organic Solar Cells. Advanced Functional Materials, 2021, 31, 2010535.	7.8	55
9	Molecular design revitalizes the low-cost PTV-polymer for highly efficient organic solar cells. National Science Review, 2021, 8, nwab031.	4.6	70
10	Theoretical analysis of the adsorption of phosphoric acid and model phosphate monoesters on CeO2(111). Surface Science, 2021, 705, 121776.	0.8	6
11	A New Conjugated Polymer that Enables the Integration of Photovoltaic and Lightâ€Emitting Functions in One Device. Advanced Materials, 2021, 33, e2101090.	11.1	129
12	Simultaneous Improvement of Efficiency and Stability of Organic Photovoltaic Cells by using a Crossâ€Linkable Fullerene Derivative. Small, 2021, 17, e2101133.	5.2	34
13	Rational Anode Engineering Enables Progresses for Different Types of Organic Solar Cells. Advanced Energy Materials, 2021, 11, 2100492.	10.2	108
14	Elucidating the Mechanism of Ambient-Temperature Aldol Condensation of Acetaldehyde on Ceria. ACS Catalysis, 2021, 11, 8621-8634.	5.5	14
15	Impact of Electrostatic Interaction on Bulk Morphology in Efficient Donorâ€“Acceptor Photovoltaic Blends. Angewandte Chemie - International Edition, 2021, 60, 15988-15994.	7.2	60
16	Impact of Electrostatic Interaction on Bulk Morphology in Efficient Donorâ€“Acceptor Photovoltaic Blends. Angewandte Chemie, 2021, 133, 16124-16130.	1.6	11
17	Oxygen electrochemistry in Liâ€O₂ batteries probed by in situ surfaceâ€enhanced Raman spectroscopy. SusMat, 2021, 1, 345-358.	7.8	31
18	CoCrFeNi High-Entropy Alloy as an Enhanced Hydrogen Evolution Catalyst in an Acidic Solution. Journal of Physical Chemistry C, 2021, 125, 17008-17018.	1.5	25

#	Article	IF	Citations
19	Squaraine organic crystals with strong dipole effect toward stable lithium-organic batteries. Energy Storage Materials, 2021, 41, 240-247.	9.5	16
20	Thermoplastic Elastomer Tunes Phase Structure and Promotes Stretchability of Highâ€Efficiency Organic Solar Cells. Advanced Materials, 2021, 33, e2106732.	11.1	101
21	The effect of aggregation behavior on photovoltaic performances in benzodithiophene-thiazolothiazole-based wide band-gap conjugated polymers with side chain position changes. Polymer Chemistry, 2020, 11, 1629-1636.	1.9	30
22	Strain Effect in Palladium Nanostructures as Nanozymes. Nano Letters, 2020, 20, 272-277.	4.5	85
23	Adsorption structure of adenine on cerium oxide. Applied Surface Science, 2020, 530, 147257.	3.1	8
24	Quantifying V_{oc} loss induced by alkyl pendants of acceptors in organic solar cells. Journal of Materials Chemistry C, 2020, 8, 12568-12577.	2.7	14
25	Catalytic Encounters at the Molecular Level: Gabor A. Somorjai Award Symposium for Creative Research in Catalysis in Honor of Professor Manos Mavrikakis. Topics in Catalysis, 2020, 63, 617-617.	1.3	0
26	Hydrogen Adsorption on Ordered and Disordered Pt-Ni Alloys. Topics in Catalysis, 2020, 63, 714-727.	1.3	4
27	Low Temperature Aggregation Transitions in N3 and Y6 Acceptors Enable Doubleâ€Annealing Method That Yields Hierarchical Morphology and Superior Efficiency in Nonfullerene Organic Solar Cells. Advanced Functional Materials, 2020, 30, 2005011.	7.8	66
28	Reduced Nonradiative Recombination Energy Loss Enabled Efficient Polymer Solar Cells via Tuning Alkyl Chain Positions on Pendent Benzene Units of Polymers. ACS Applied Materials & Interfaces, 2020, 12, 24184-24191.	4.0	7
29	Efficient charge generation at low energy losses in organic solar cells: a key issues review. Reports on Progress in Physics, 2020, 83, 082601.	8.1	43
30	Efficient Exciton Dissociation Enabled by the End Group Modification in Non-Fullerene Acceptors. Journal of Physical Chemistry C, 2020, 124, 7691-7698.	1.5	18
31	Tuning the Hybridization of Local Exciton and Chargeâ€Transfer States in Highly Efficient Organic Photovoltaic Cells. Angewandte Chemie - International Edition, 2020, 59, 9004-9010.	7.2	144
32	Recent Progress in Chlorinated Organic Photovoltaic Materials. Accounts of Chemical Research, 2020, 53, 822-832.	7.6	198
33	Singleâ€Junction Organic Photovoltaic Cells with Approaching 18% Efficiency. Advanced Materials, 2020, 32, e1908205.	11.1	1,407
34	Tuning the Hybridization of Local Exciton and Chargeâ€Transfer States in Highly Efficient Organic Photovoltaic Cells. Angewandte Chemie, 2020, 132, 9089-9095.	1.6	24
35	Ecoâ€Compatible Solventâ€Processed Organic Photovoltaic Cells with Over 16% Efficiency. Advanced Materials, 2019, 31, e1903441.	11.1	445
36	Wide-gap non-fullerene acceptor enabling high-performance organic photovoltaic cells for indoor applications. Nature Energy, 2019, 4, 768-775.	19.8	407

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37	Reduced Nonradiative Energy Loss Caused by Aggregation of Nonfullerene Acceptor in Organic Solar Cells. Advanced Energy Materials, 2019, 9, 1901823.	10.2	72
38	Investigating the Trade-Off between Device Performance and Energy Loss in Nonfullerene Organic Solar Cells. ACS Applied Materials & Interfaces, 2019, 11, 29124-29131.	4.0	24
39	Bioalcohol production from acidogenic products via a two-step process: A case study of butyric acid to butanol. Applied Energy, 2019, 252, 113482.	5.1	47
40	p-Doped Conducting Polyelectrolyte as an Anode Interlayer Enables High Efficiency for 1 cm² Printed Organic Solar Cells. ACS Applied Materials & Interfaces, 2019, 11, 20205-20213.	4.0	28
41	14.7% Efficiency Organic Photovoltaic Cells Enabled by Active Materials with a Large Electrostatic Potential Difference. Journal of the American Chemical Society, 2019, 141, 7743-7750.	6.6	379
42	CO₂ electrochemical reduction at thiolate-modified bulk Au electrodes. Catalysis Science and Technology, 2019, 9, 2689-2701.	2.1	22
43	Enhanced Ï€â€“Ï€ Interactions of Nonfullerene Acceptors by Volatilizable Solid Additives in Efficient Polymer Solar Cells. Advanced Materials, 2019, 31, e1900477.	11.1	99
44	Efficiency enhancements of a restricted stochastic search algorithm for locating local and global minima. Chemical Physics Letters, 2019, 725, 1-7.	1.2	0
45	Significant Effect of Fluorination on Simultaneously Improving Work Function and Transparency of Anode Interlayer for Organic Solar Cells. Advanced Energy Materials, 2019, 9, 1803826.	10.2	21
46	Reaction pathways for HCN on transition metal surfaces. Physical Chemistry Chemical Physics, 2019, 21, 5274-5284.	1.3	4
47	Achieving Over 15% Efficiency in Organic Photovoltaic Cells via Copolymer Design. Advanced Materials, 2019, 31, e1808356.	11.1	388
48	Defect engineering activating (Boosting) zinc storage capacity of MoS2. Energy Storage Materials, 2019, 16, 527-534.	9.5	199
49	Recent Advances in Fullereneâ€free Polymer Solar Cells: Materials and Devices. Chinese Journal of Chemistry, 2019, 37, 207-215.	2.6	46
50	Coupling of Acetaldehyde to Crotonaldehyde on CeO_{2â€“x}(111): Bifunctional Mechanism and Role of Oxygen Vacancies. Journal of Physical Chemistry C, 2019, 123, 8273-8286.	1.5	23
51	Theoretical Investigation of the Effects of Metal Cations on Oxygen Reduction Reaction in Non-Aqueous Li-Air Batteries. ECS Meeting Abstracts, 2019, , .	0.0	0
52	An experimental and theoretical study of adenine adsorption on Au(111). Physical Chemistry Chemical Physics, 2018, 20, 4688-4698.	1.3	13
53	Theoretical investigation of dephosphorylation of phosphate monoesters on CeO2(111). Catalysis Today, 2018, 312, 141-148.	2.2	16
54	Multi-component non-fullerene acceptors with tunable bandgap structures for efficient organic solar cells. Journal of Materials Chemistry A, 2018, 6, 23644-23649.	5.2	47

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55	Enhancing the Photovoltaic Performance of Nonfullerene Acceptors via Conjugated Rotatable End Groups. Advanced Energy Materials, 2018, 8, 1802131.	10.2	24
56	Printable MoO_x Anode Interlayers for Organic Solar Cells. Advanced Materials, 2018, 30, e1801718.	11.1	71
57	Mechanistic Insights into Oxygen Reduction Reactions in Non-Aqueous Metal-Air Batteries. ECS Meeting Abstracts, 2018, , .	0.0	0
58	DFT-Based Method for More Accurate Adsorption Energies: An Adaptive Sum of Energies from RPBE and vdW Density Functionals. Journal of Physical Chemistry C, 2017, 121, 4937-4945.	1.5	80
59	Mechanistic origin of low polarization in aprotic Naâ€“O₂ batteries. Physical Chemistry Chemical Physics, 2017, 19, 12375-12383.	1.3	24
60	Estimation of electric field effects on the adsorption of molecular superoxide species on Au based on density functional theory. Physical Chemistry Chemical Physics, 2017, 19, 32626-32635.	1.3	8
61	Covalent versus localized nature of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>4</mml:mn><mml:mi>f</mml:mi></mml:mrow></mml:m electrons in ceria: Resonant angle-resolved photoemission spectroscopy and density functional theory. Physical Review B, 2017, 95, .	1.1	13
62	Adsorption of transition metal adatoms on h-BN/Rh(111): Implications for nanocluster self-assembly. Catalysis Today, 2017, 280, 220-231.	2.2	15
63	Simulated Temperature Programmed Desorption of Acetaldehyde on CeO2(111): Evidence for the Role of Oxygen Vacancy and Hydrogen Transfer. Topics in Catalysis, 2017, 60, 446-458.	1.3	15
64	Theoretical Investigation of Oxygen- and Bromine-Functionalized Model Carbon Structures for Li-Redox Activity. ECS Meeting Abstracts, 2017, , .	0.0	0
65	Hydrogenation at Metal-Ligand Interfaces in CO2 Electrochemical Reduction. ECS Meeting Abstracts, 2017, , .	0.0	0
66	Mechanistic Insights into Oxygen Reduction and Evolution Reactions in Non-Aqueous Metal-Air Batteries. ECS Meeting Abstracts, 2017, , .	0.0	0
67	Interaction of Thiol Ligands with Gold in Electrocatalytic CO2 Reduction. ECS Meeting Abstracts, 2017, , .	0.0	0
68	CO Adsorption on Au Nanoparticles Grown on Hexagonal Boron Nitride/Rh(111). Journal of Physical Chemistry C, 2016, 120, 10909-10918.	1.5	27
69	Amorphous Li₂O₂: Chemical Synthesis and Electrochemical Properties. Angewandte Chemie - International Edition, 2016, 55, 10717-10721.	7.2	135
70	Amorphous Li₂O₂: Chemical Synthesis and Electrochemical Properties. Angewandte Chemie, 2016, 128, 10875-10879.	1.6	37
71	Spectroscopic Identification of the Auâ€“C Bond Formation upon Electroreduction of an Aryl Diazonium Salt on Gold. Langmuir, 2016, 32, 11514-11519.	1.6	14
72	Potential-Dependent Generation of O₂^{â€“} and LiO₂ and Their Critical Roles in O₂ Reduction to Li₂O₂ in Aprotic Liâ€“O₂ Batteries. Journal of Physical Chemistry C, 2016, 120, 3690-3698.	1.5	149

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73	Role of Superoxide Anion in the Oxygen Reduction Reaction in Non-Aqueous Electrolytes with a Proton or Lithium Source. ECS Meeting Abstracts, 2016, , .	0.0	0
74	Theoretical Investigation of the Oxygen Reduction Reaction in Non-Aqueous Electrolytes. ECS Meeting Abstracts, 2016, , .	0.0	0
75	Enhanced Electrocatalytic CO2 Reduction on Thiol-Functionalized Gold. ECS Meeting Abstracts, 2016, , .	0.0	0
76	Tuning the Selectivity of CO2 Electrochemical Reduction Toward Hydrocarbon with Ligand Modified Metal Electrocatalyst. ECS Meeting Abstracts, 2016, , .	0.0	0
77	Direct Detection of the Superoxide Anion as a Stable Intermediate in the Electroreduction of Oxygen in a Nonâ€Aqueous Electrolyte Containing Phenol as a Proton Source. Angewandte Chemie, 2015, 127, 8283-8286.	1.6	19
78	Direct Detection of the Superoxide Anion as a Stable Intermediate in the Electroreduction of Oxygen in a Nonâ€Aqueous Electrolyte Containing Phenol as a Proton Source. Angewandte Chemie - International Edition, 2015, 54, 8165-8168.	7.2	78
79	Reconciling the electronic and geometric corrugations of the hexagonal boron nitride and graphene nanomeshes. Surface Science, 2015, 642, L16-L19.	0.8	9
80	Reactivity and reaction intermediates for acetic acid adsorbed on CeO2(1 1 1). Catalysis Today, 2015, 253, 65-76.	2.2	43
81	Reversibility of Noble Metal-Catalyzed Aprotic Li-O₂ Batteries. Nano Letters, 2015, 15, 8084-8090.	4.5	165
82	Unlocking the energy capabilities of micron-sized LiFePO4. Nature Communications, 2015, 6, 7898.	5.8	65
83	Pdâ€“Ir Coreâ€“Shell Nanocubes: A Type of Highly Efficient and Versatile Peroxidase Mimic. ACS Nano, 2015, 9, 9994-10004.	7.3	254
84	Propane Ammoxidation over Moâ€“Vâ€“Teâ€“Nbâ€“O M1 Phase Investigated by DFT: Elementary Steps of Ammonia Adsorption, Activation and NH Insertion into Ï€-Allyl Intermediate. Topics in Catalysis, 2014, 57, 1145-1151.	1.3	11
85	Formation and stability of dense arrays of Au nanoclusters on hexagonal boron nitride/Rh(111). Physical Review B, 2014, 89, .	1.1	29
86	Energetics of Adsorbed CH₂ and CH on Pt(111) by Calorimetry: The Dissociative Adsorption of Diiodomethane. Journal of Physical Chemistry C, 2014, 118, 29310-29321.	1.5	13
87	Catalytically active Au-O(OH) _x - species stabilized by alkali ions on zeolites and mesoporous oxides. Science, 2014, 346, 1498-1501.	6.0	544
88	Propane ammoxidation over Moâ€“Vâ€“Teâ€“Nbâ€“O M1 phase: Density functional theory study of propane oxidative dehydrogenation steps. Catalysis Today, 2014, 238, 28-34.	2.2	21
89	Identifying Active Functionalities on Fewâ€Layered Graphene Catalysts for Oxidative Dehydrogenation of Isobutane. ChemSusChem, 2014, 7, 483-491.	3.6	56
90	Adsorption Energy of tert-Butyl on Pt(111) by Dissociation of tert-Butyl Iodide: Calorimetry and DFT. Journal of Physical Chemistry C, 2014, 118, 427-438.	1.5	22

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91	Effects of hydrogen and water on the activity and selectivity of acetic acid hydrogenation on ruthenium. Green Chemistry, 2014, 16, 911-924.	4.6	49
92	Synthesis, Characterization, and Computation of Catalysts at the Center for Atomic-Level Catalyst Design. Journal of Physical Chemistry C, 2014, 118, 20043-20069.	1.5	21
93	Adsorption and Diffusion of 4d and 5d Transition Metal Adatoms on Graphene/Ru(0001) and the Implications for Cluster Nucleation. Topics in Catalysis, 2014, 57, 69-79.	1.3	28
94	Graphene moirÃ© structure grown on a pseudomorphic metal overlayer supported on Ru(0001). Surface Science, 2013, 611, 67-73.	0.8	17
95	High-throughput screening of monometallic catalysts for aqueous-phase hydrogenation of biomass-derived oxygenates. Applied Catalysis B: Environmental, 2013, 140-141, 98-107.	10.8	78
96	Adsorption and diffusion of the Rh and Au adatom on graphene moirÃ©/Ru(0001). Journal of Chemical Physics, 2013, 138, 184710.	1.2	22
97	A combined HAADF STEM and density functional theory study of tantalum and niobium locations in the Moâ€“Vâ€“Teâ€“Ta(Nb)â€“O M1 phases. Catalysis Communications, 2012, 29, 68-72.	1.6	19
98	Oxygen Vacancy-Assisted Coupling and Enolization of Acetaldehyde on CeO₂(111). Journal of the American Chemical Society, 2012, 134, 18034-18045.	6.6	97
99	Trends in the Catalytic Activity of Transition Metals for the Oxygen Reduction Reaction by Lithium. Journal of Physical Chemistry Letters, 2012, 3, 891-895.	2.1	75
100	Decomposition of Furan on Pd(111). Topics in Catalysis, 2012, 55, 290-299.	1.3	13
101	Exploring the structure and chemical activity of 2-D gold islands on graphene moirÃ©/Ru(0001). Faraday Discussions, 2011, 152, 267.	1.6	37
102	Oxygen Reduction by Lithium on Model Carbon and Oxidized Carbon Structures. Journal of the Electrochemical Society, 2011, 158, A1177.	1.3	66
103	Propane Ammoxidation Over the Moâ€“Vâ€“Teâ€“Nbâ€“O M1 Phase: Reactivity of Surface Cations in Hydrogen Abstraction Steps. Topics in Catalysis, 2011, 54, 605-613.	1.3	24
104	Effect of Pd surface structure on the activation of methyl acetate. Catalysis Today, 2011, 165, 96-105.	2.2	17
105	Aqueousâ€Phase Hydrogenation of Acetic Acid over Transition Metal Catalysts. ChemCatChem, 2010, 2, 1420-1424.	1.8	123
106	Activation of methyl acetate on Pd(111). Surface Science, 2010, 604, 887-892.	0.8	23
107	Partial and complete reduction of O2 by hydrogen on transition metal surfaces. Surface Science, 2010, 604, 1565-1575.	0.8	189
108	Adsorption of Propane, Isopropyl, and Hydrogen on Cluster Models of the M1 Phase of Moâ^'Vâ^'Teâ^'Nbâ^'O Mixed Metal Oxide Catalyst. Journal of Physical Chemistry C, 2010, 114, 4544-4549.	1.5	28

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109	O 2 reduction by lithium on Au(111) and Pt(111). Journal of Chemical Physics, 2010, 133, 024703.	1.2	88
110	Temperature evolution of structure and bonding of formic acid and formate on fully oxidized and highly reduced CeO2(111). Physical Chemistry Chemical Physics, 2009, 11, 11171.	1.3	61
111	Thermodynamics of Environment-Dependent Oxygen Chemisorption on Pt(111). Journal of Physical Chemistry C, 2008, 112, 9559-9572.	1.5	173
112	A first-principles investigation of the effect of Pt cluster size on CO and NO oxidation intermediates and energetics. Physical Chemistry Chemical Physics, 2008, 10, 6009.	1.3	45
113	Bimetallic and Ternary Alloys for Improved Oxygen Reduction Catalysis. Topics in Catalysis, 2007, 46, 276-284.	1.3	202
114	The Effect of Coadsorbed Oxygen on the Adsorption and Diffusion of Potassium on Rh(110):â€‰ A First-Principles Study. Journal of Physical Chemistry C, 2007, 111, 7446-7455.	1.5	12
115	Lattice strain effects on CO oxidation on Pt(111). Physical Chemistry Chemical Physics, 2006, 8, 3369.	1.3	96
116	Effect of Particle Size on the Oxidizability of Platinum Clusters. Journal of Physical Chemistry A, 2006, 110, 5839-5846.	1.1	75
117	Thermodynamic Equilibrium Compositions, Structures, and Reaction Energies of PtxOy(x= 1â^'3) Clusters Predicted from First Principles. Journal of Physical Chemistry B, 2006, 110, 16591-16599.	1.2	51
118	Theoretical Aspects of Oxide Particle Stability and Chemical Reactivity. , 2006, , 289-309.		0
119	Effect of Subsurface Oxygen on the Reactivity of the Ag(111) Surface. Journal of the American Chemical Society, 2005, 127, 12823-12827.	6.6	151
120	Controlling the Catalytic Activity of Platinum-Monolayer Electrocatalysts for Oxygen Reduction with Different Substrates. Angewandte Chemie - International Edition, 2005, 44, 2132-2135.	7.2	1,015
121	Atomic and molecular adsorption on Pt(111). Surface Science, 2005, 587, 159-174.	0.8	247
122	On the origin of the catalytic activity of gold nanoparticles for low-temperature CO oxidation. Journal of Catalysis, 2004, 223, 232-235.	3.1	1,122
123	Adsorption and Dissociation of O2on Ptâ^'Co and Ptâ^'Fe Alloys. Journal of the American Chemical Society, 2004, 126, 4717-4725.	6.6	615
124	The adsorption and dissociation of O 2 molecular precursors on Cu: the effect of steps. Surface Science, 2003, 538, 219-232.	0.8	47
125	Adsorption and Dissociation of O2on Gold Surfaces:Â Effect of Steps and Strain. Journal of Physical Chemistry B, 2003, 107, 9298-9307.	1.2	322
126	Adsorption and dissociation of O2 on Ir(111). Journal of Chemical Physics, 2002, 116, 10846-10853.	1.2	67

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127	Universality in Heterogeneous Catalysis. Journal of Catalysis, 2002, 209, 275-278.	3.1	1,167
128	Adsorption and dissociation of O2 on Cu(): thermochemistry, reaction barrier and the effect of strain. Surface Science, 2001, 494, 131-144.	0.8	175
129	Recent Developments in the Electrocatalysis of the O2 Reduction Reaction. , 0, , 271-315.		10
130	Squaraine Organic Crystals with Strong Dipole Effect Toward Stable Lithium-Organic Batteries. SSRN Electronic Journal, 0, , .	0.4	0